Directionally Unsplit Riemann-solverbased Hydrodynamic Schemes in Heterogeneous GPU Computing

Hsi-Yu Schive (薛熙于)

Graduate Institute of Physics, National Taiwan University
Leung Center for Cosmology and Particle Astrophysics (LeCosPA)

Ui-Han Zhang (張瑋瀚), Tzihong Chiueh (闕志鴻),

Graduate Institute of Physics, National Taiwan University

Leung Center for Cosmology and Particle Astrophysics (LeCosPA)

Manycore and Accelerator-based High-performance Scientific Computing Workshop (27/01/2011 in ICCS)

Outline

- Introduction to GAMER
 - ◆ GPU-accelerated Adaptive-MEsh-Refinement Code for Astrophysics
 - Previous benchmark results
- Directionally unsplit hydro schemes
 - MUSCL-Hancock Method (MHM)
 - Corner-Transport-Upwind (CTU)
- Optimization and performance
 - Uniform mesh
 - Adaptive mesh refinement
- Conclusion and future work

Previous Works

- GraCCA system (2006)
 - Graphic-Card Cluster for Astrophysics
 - ◆ 16 nodes, 32 GPUs (GeForce 8800 GTX)
 - ♦ Peak performance: 16.2 TFLOPS
- Parallel direct N-body simulation in GraCCA
 - Individual time-step
 - ◆ 4th order Hermite integrator
 - ♦ 7.1 TFLOPS
 - ◆ GPU/CPU speed-up ~ 200



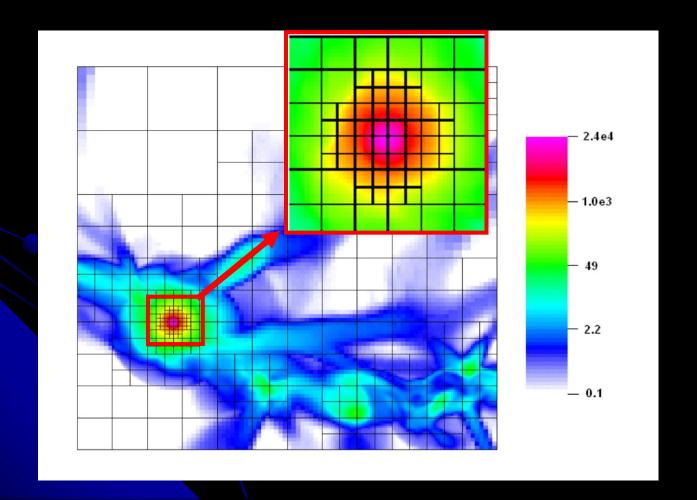
◆Ref: Schive, H-Y., et al. 2008, NewA, 13, 418

GAMER

GPU-accelerated Adaptive-MEsh-Refinement Code for Astrophysics

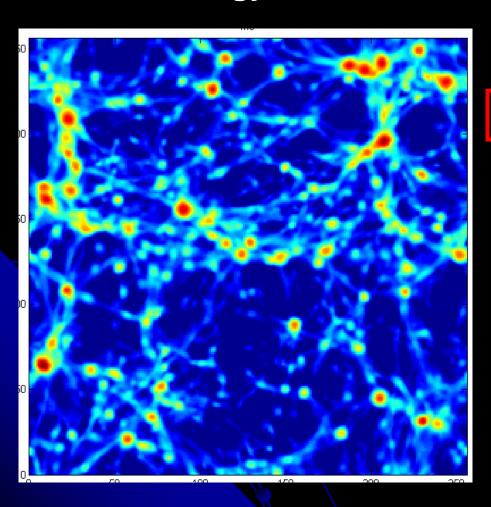
Adaptive-Mesh-Refinement (AMR)

- Resolution adaptively changes with space and time
- Flexible refinement criteria



AMR Example

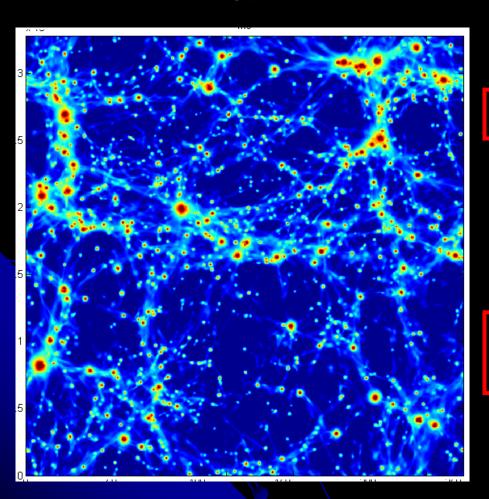
Cosmology simulations with different refinement levels



Base level 2563, Refined level 0

AMR Example

Cosmology simulations with different refinement levels



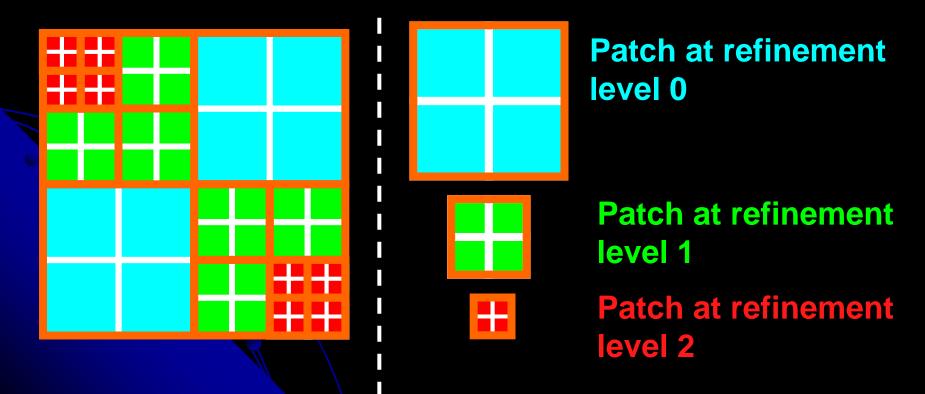
Base level 2563, Refined level 0



Base level 256³, Refined level 5 (effective resolution = 8192³)

AMR Scheme in GAMER

- ◆Refinement unit : patch (containing a fixed number of cells, e.g., 8³)
- **◆Support GPU hydro and gravity solvers**
- ◆ Hierarchical oct-tree data structure



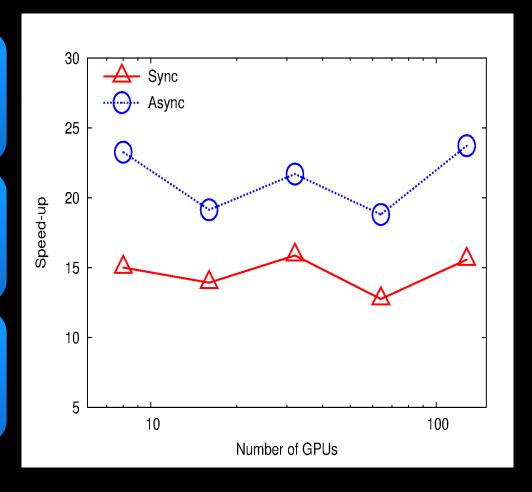
Benchmark Test: NAOC GPU Cluster (Laohu)

National Astronomical Observatories, Chinese Academy of Sciences

1 - 128 Tesla C1060 vs.

1 - 128 Xeon E5520 cores

Speed-up is measured in one-GPU-to-one-CPU-core basis



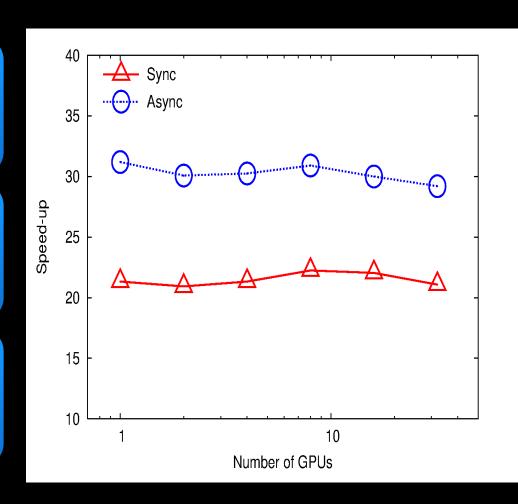
Benchmark Test: NERSC GPU Cluster (Dirac)

National Energy Research Scientific Computing Center

1 – 32 Tesla C2050 vs.

1 - 32 Xeon E5530 cores

Speed-up is measured in one-GPU-to-one-CPU-core basis

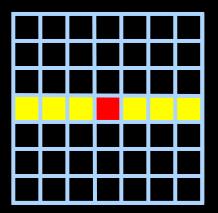


Directionally Unsplit Hydro Schemes

Splitting vs. Unsplitting

Splitting methods:

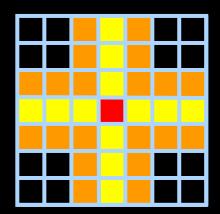
- 3D update : x→y→z
- 1D stencil



- GPU shared memory
 - straightforward
- Supported schemes in GAMER
 - Relaxing TVD (RTVD)
 - Weighted-Averaged-Flux (WAF)

Unsplitting methods:

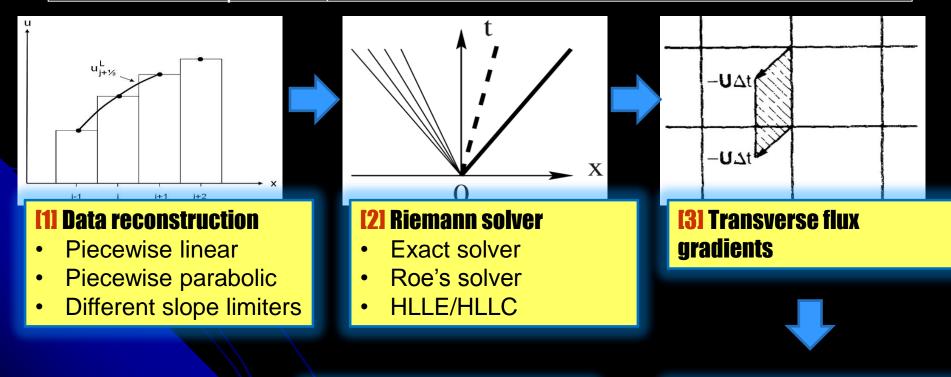
- 3D update : x + y + z
- 3D stencil



- GPU shared memory→ non-trivial
- Supported schemes in GAMER
 - MUSCL-Hancock Method (MHM)
 - MUSCL-Hancock with Riemann prediction (MHMRP)
 - Corner-Transport-Upwind (CTU)

Corner-Transport-Upwind (CTU)

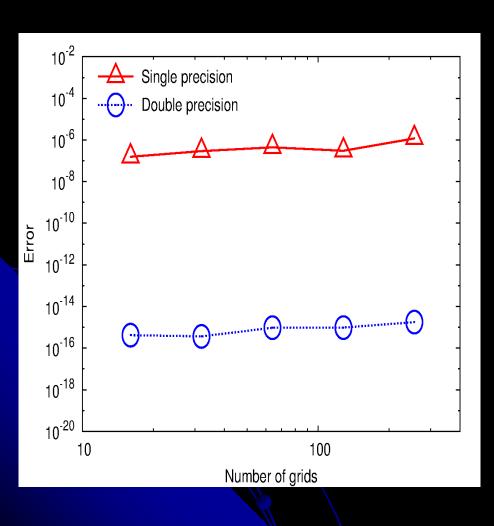
- Colella, P., 1990. J. Comput. Phys. 87, 171.
- Extended to MHD and well tested in Athena code
 - Stone, J.M., Gardiner, T.A., Teuben, P., Hawley, J.F., Simon, J.B., 2008. ApJS 178, 137.



l Riemann solver

(5) Update solution

Accuracy Compared to Athena



Athena:

Widely-adopted MHD/Hydro code (https://trac.princeton.edu/Athena/)
Developed by James M. Stone

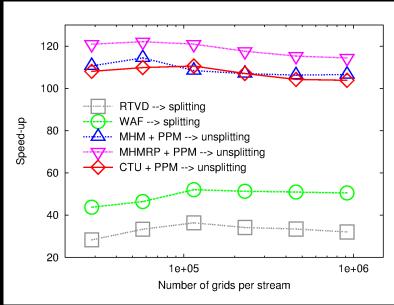
Test problem : Blast-wave test

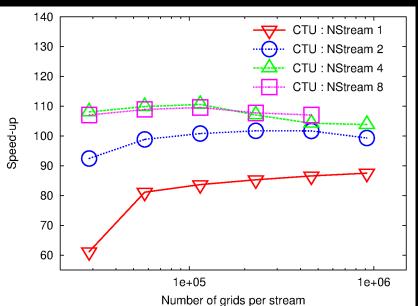
$$\mathsf{Error} = \frac{|\rho_{Athena} - \rho_{GAMER}|}{\rho_{Athena}}$$

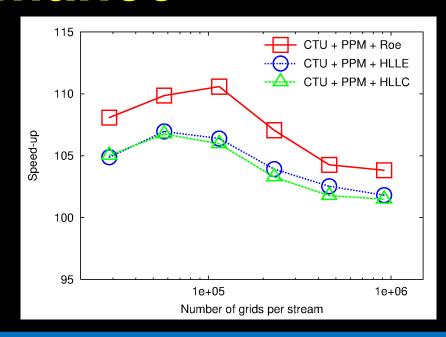
Error_{single}: $10^{-6} \sim 10^{-7}$

Error_{double}: 10⁻¹⁵~10⁻¹⁶

Performance







Splitting schemes → shared memory Unsplitting schemes → global memory

CUDA stream : PCI-E / computation overlap

Speed-up: 110x ~ 120x

(vs. 1 CPU core)

Optimization and Performance in GAMER

Optimization in GAMER

I11 PCI-E data transfer & GPU computation overlap

GPU computation (hydro/gravity solver)

Concurrency

= **Performance**

Data : CPU → GPU

Data : GPU → CPU

Prepare the input data (interpolation & memory copy)

Handle the output data (fit into oct-tree)

Coarse-grid correction & grid refinement

Optimization in GAMER

[2] GPU & CPU overlap

GPU computation & CPU⇔GPU data transfer

Prepare the input data (Interpolation & Memory copy)

Handle the output data (fit into oct-tree)

Coarse-grid correction & Grid refinement

Optimization in GAMER

[3] OpenMP parallelization

[CPU] Prepare the input data

OpenMP Thread 1
OpenMP Thread 2

[GPU] GPU computation & CPU⇔GPU data transfer

OpenMP Thread N

[CPU] Handle the output data

OpenMP Thread 1 OpenMP Thread 2

OpenMP Thread N

11

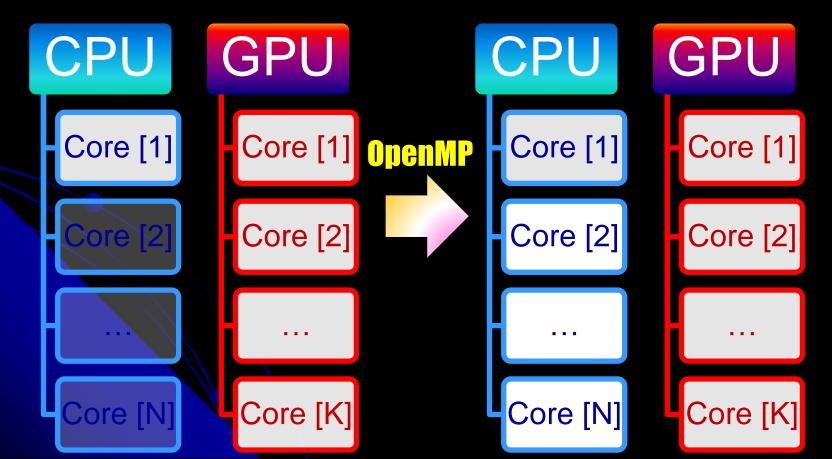
[CPU] Coarse-grid correction & Grid refinement

OpenMP Thread 1 OpenMP Thread 2

OpenMP Thread N

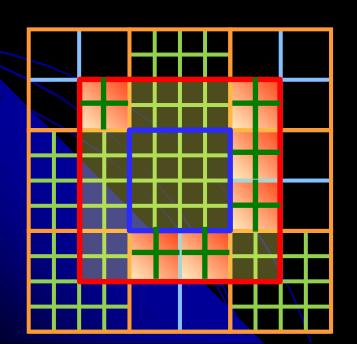
OpenMP in GAMER

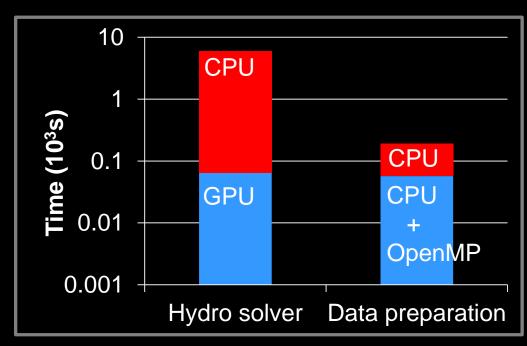
- Fully exploit the multi-core CPU computing power
 - ♦ N GPUs + K CPU cores (N≠K)



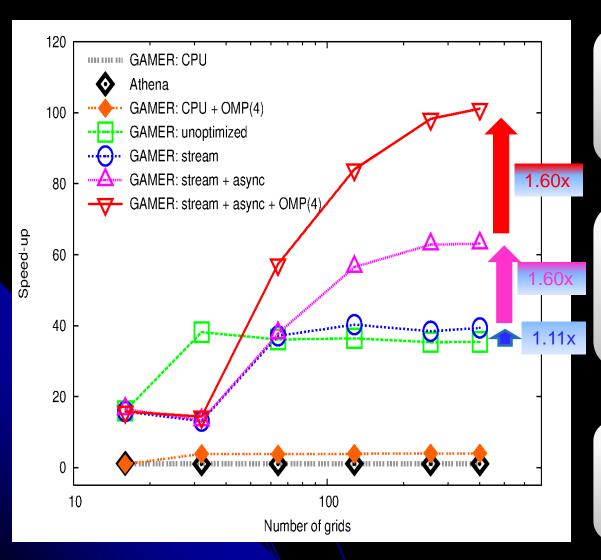
OpenMP in GAMER

- Performance can be significantly improved in GAMER
 - ◆ Using CPU to prepare the input data for GPU is extremely time-consuming
 - ◆ Performance bottleneck : 1.5x~3.0x longer than GPU calculation





Uniform-mesh Performance



GPU: 1 NVIDIA Tesla C2050

CPU: 1 Intel Xeon E5530

Stream : PCI-E/GPU overlap

Async : CPU/GPU overlap

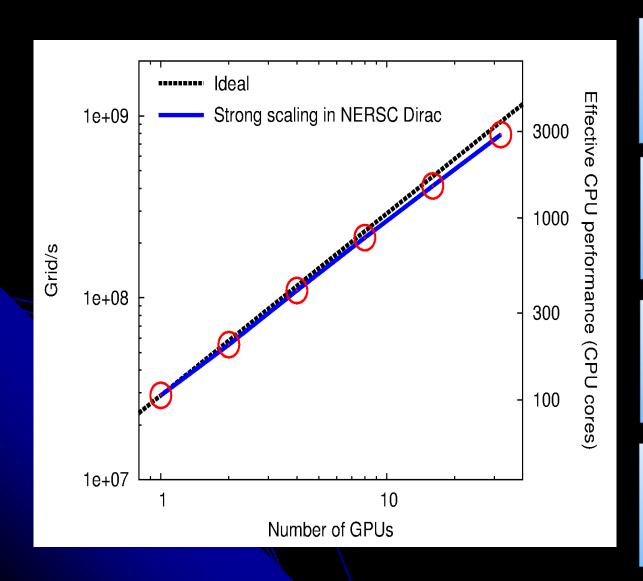
OMP(4): 4 OpenMP threads

GAMER-optimized vs.

1 CPU core : 101x

4 CPU cores: 25x

Strong Scaling



Grid Size:

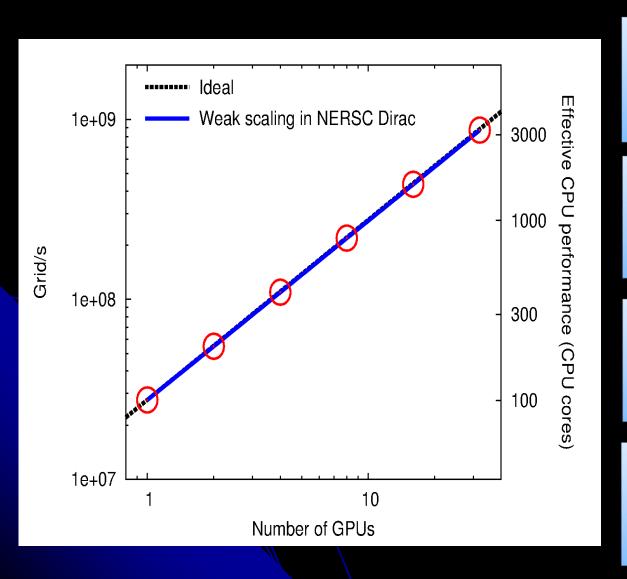
1024x1024x512

32-GPU Speed-up: **27.2**x

Equivalent to: 2,751 CPU cores

Parallel Efficiency: 85.0%

Weak Scaling



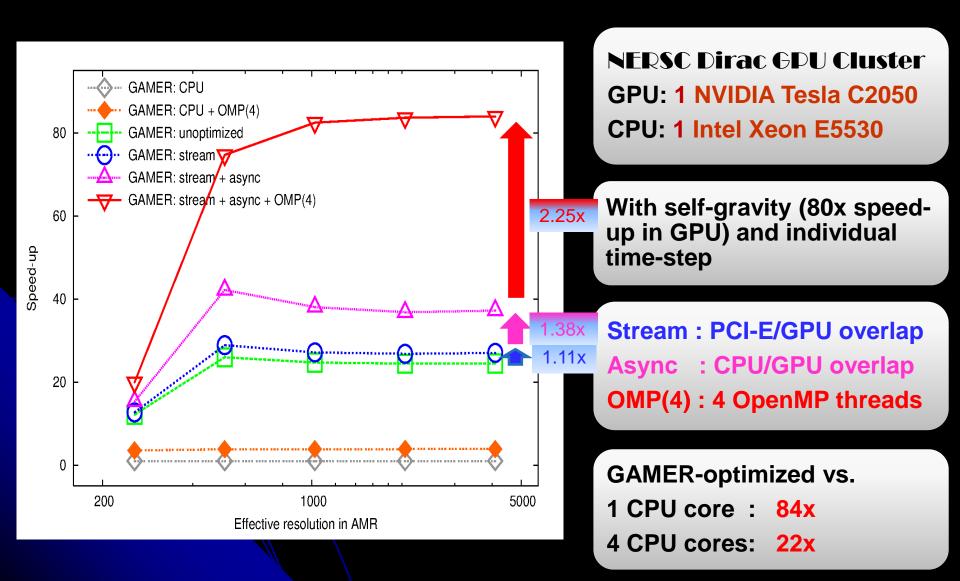
Grid Size per GPU: 512³

32-GPU Speed-up: 31.6x

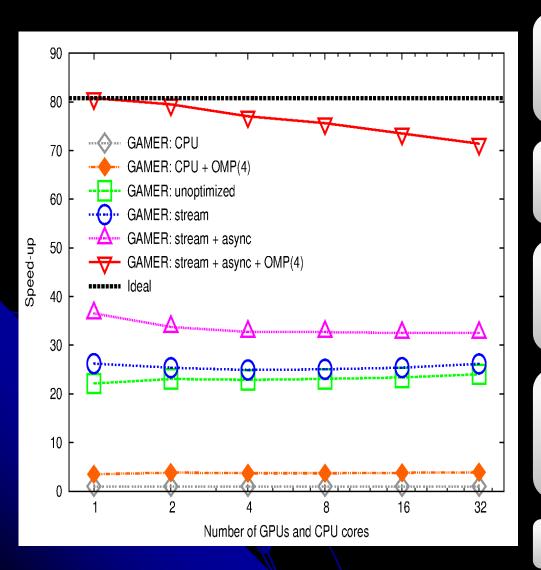
Equivalent to: 3,189 CPU cores

Parallel Efficiency: 98.8%

AMR Performance: Single GPU



AMR Performance: GPU Cluster



NERSC Dirac GPU Cluster

GPU: 1-32 NVIDIA Tesla C2050

CPU: 1-32 Intel Xeon E5530

With self-gravity (80x speed-up in GPU) and individual time-step

Stream: PCI-E/GPU overlap

Async: CPU/GPU overlap

OMP(4): 4 OpenMP threads

32 GPU vs. 32 CPU cores: **71x**

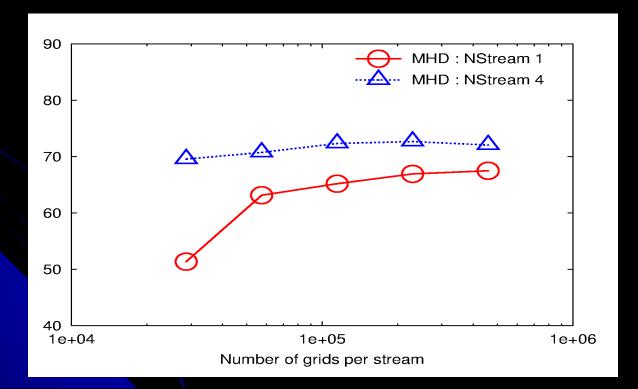
32 GPU vs. 128 CPU cores: 18x

→ Equivalent to 2,304 CPU cores

MPI \sim 11% of T_{total}

Preliminary Results in Magnetohydrodynamics (MHD)

- Corner-transport-upwind scheme
 - ◆ Piecewise linear data reconstruction
 - Roe's Riemann solver extended to MHD
- Speed-up ~ 73x (still optimizing ...)



Conclusion

- Directionally unsplit hydro schemes in GAMER:
 - ◆ Corner-Transport-Upwind & MUSCL-Hancock Method
 - ◆ MPI + OpenMP parallelization (multi CPUs + multi GPUs)
 - ◆ A framework of AMR + GPUs → general-purpose
 - ♦ 80x ~ 100x speed-up (1 GPUs vs. 1 CPU core)
 - **◆ GAMER ref : Schive, H-Y., et al. 2010, ApJS, 186, 457**
- Concurrency = Optimization
 - GPU computation
 - ◆ CPU ⇔ GPU data transfer
 - CPU computation
 - Multiple CPU cores (OpenMP)
 - ◆ Multiple GPUs (MPI)

Future Work

- More physics
 - ♦ MHD (coming soon)
 - Dark matter particles
- Overlap MPI time
- Load balance in AMR
 - ◆ Space-filling curve (Morton curve, Hilbert curve ...)
 - →Independent of the GPU implementation
- Complete analysis and visualization tools
- Desperate for more developers / users / applications
- Code request : b88202011@ntu.edu.tw